Biphenyl

92-52-4 | DTXSID4020161

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 35.7 °C

Global applicability domain: Inside

Local applicability domain index: 9.05e-01

Confidence level: 6.39e-01

Nearest Neighbors from the Training Set

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Biphenyl	Benzene, 1,1'-ethenylidenebis-	3-Methylbiphenyl
Measured: 69.0	**Measured:** 8.20	**Measured:** 4.50
Predicted: 35.7	**Predicted:** 24.9	**Predicted:** 17.9